Chemistry around AGB stars: a theoretical sensitivity study

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In collaboration with:

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Introduction

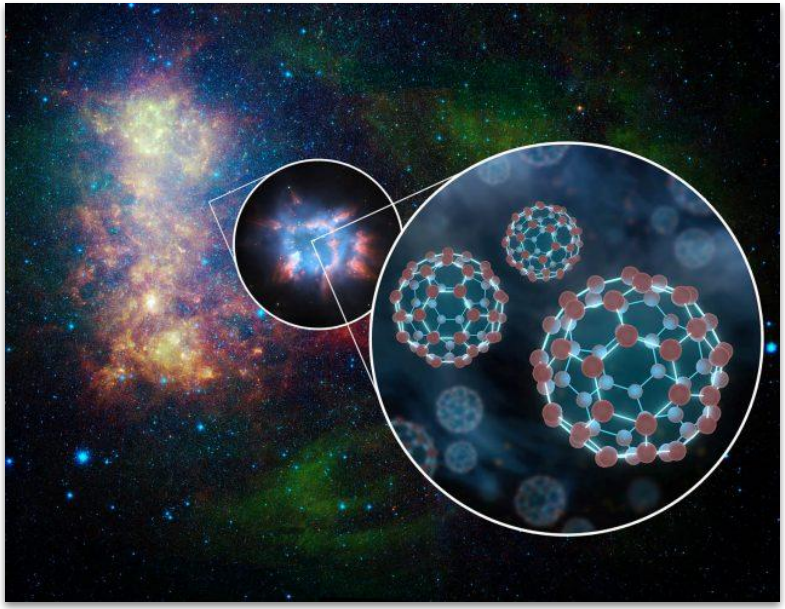
Astrochemistry

= *Study of chemical species in astrophysical environments*

Depends on:

- species present
- radiation (UV & cosmic rays)
- physical conditions

+ feedback on environment

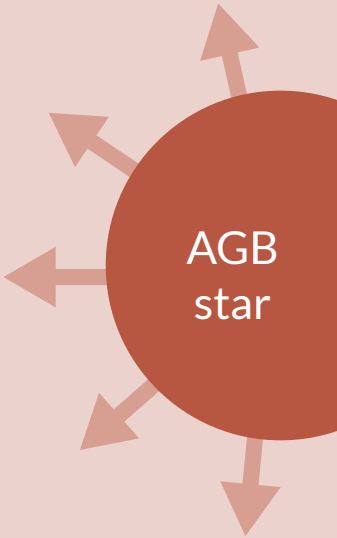


Credits: NASA/jpi-caltech/t.pyle

AGB circumstellar envelope (CSE)

- Mass loss → outflow → **large envelope**
- **Rich chemistry;**

  > 100 molecules, 15 dust species

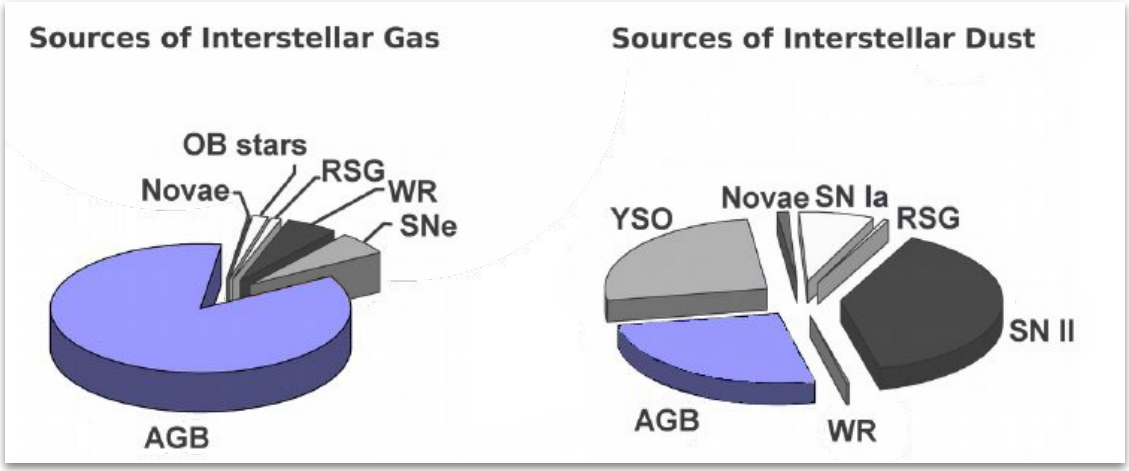


AGB circumstellar envelope (CSE)

- Mass loss → outflow → **large envelope**
- **Rich chemistry;**

  > 100 molecules, 15 dust species

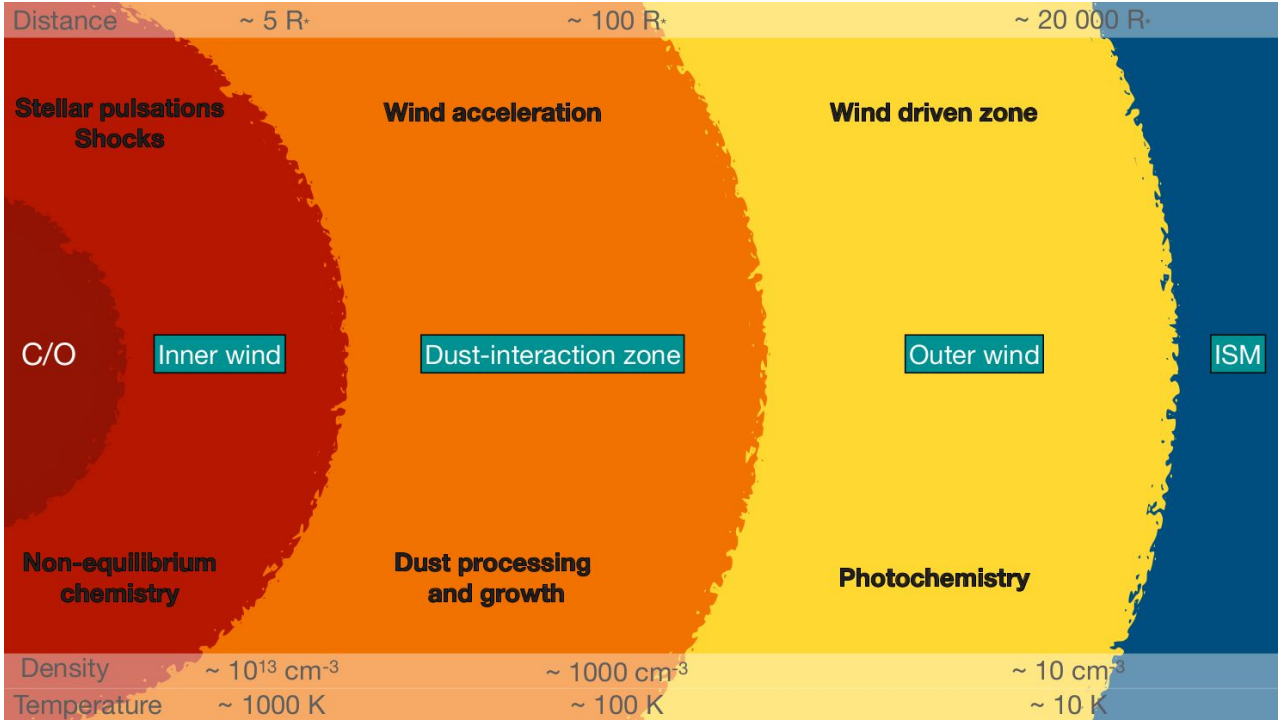
→ Enrichment of the ISM



Adapted from Tielens (2005)

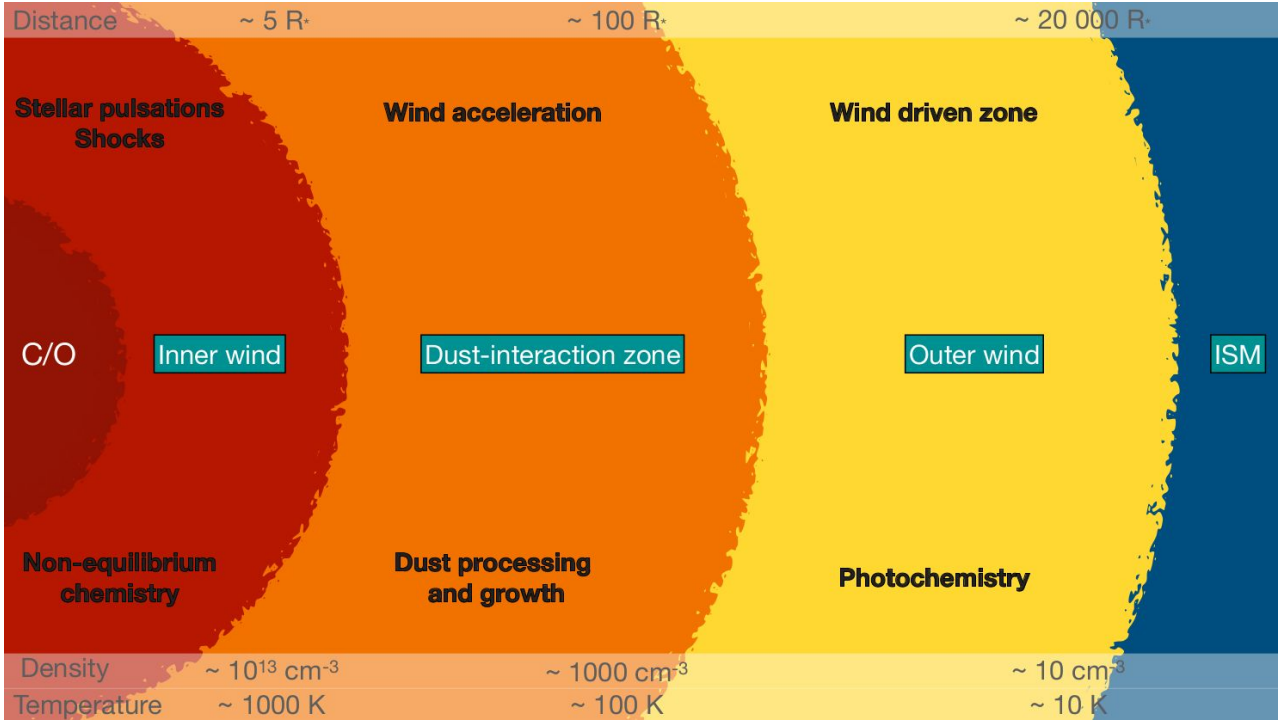
Motivation of research

AGB outflows



Source: M. Van de Sande

AGB outflows

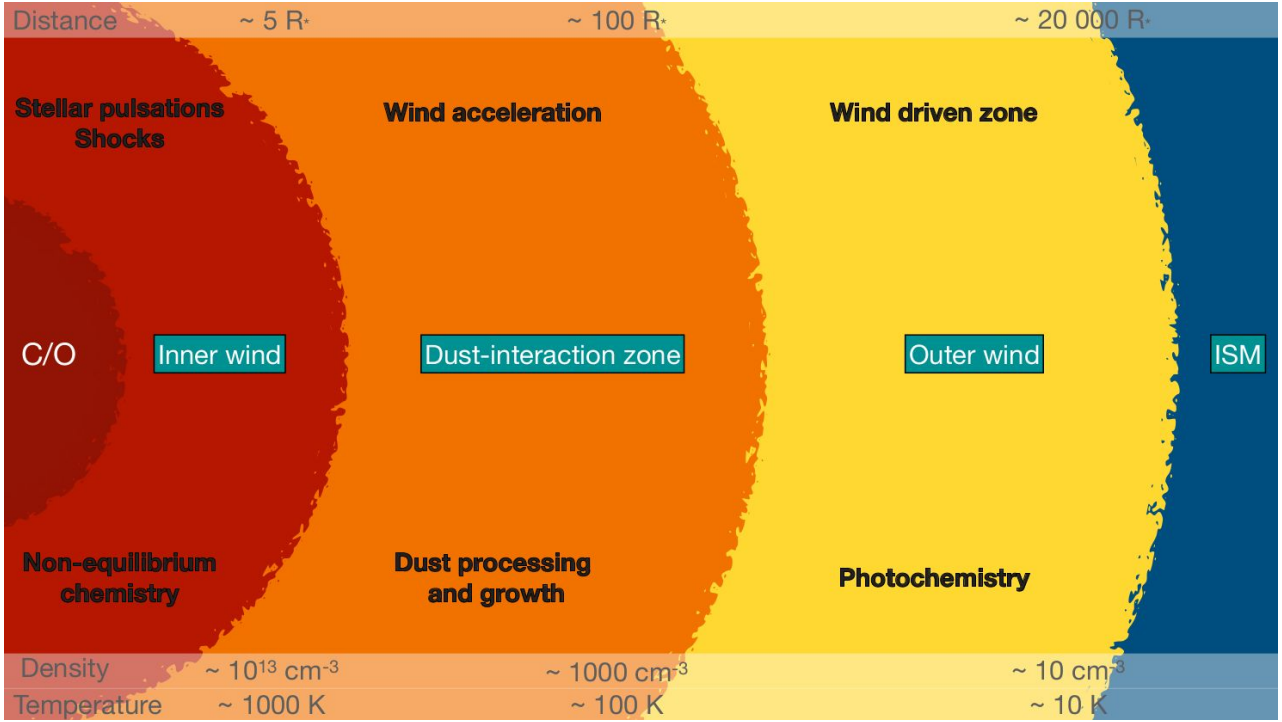


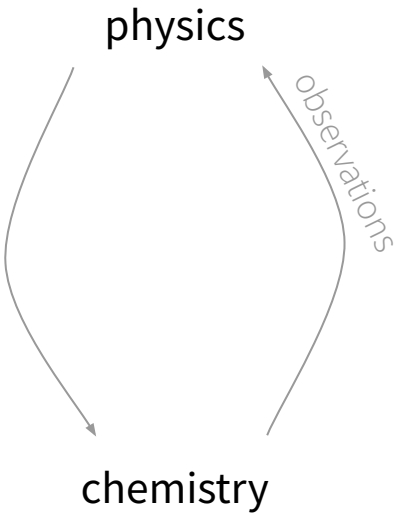
physics

chemistry

Source: M. Van de Sande

AGB outflows





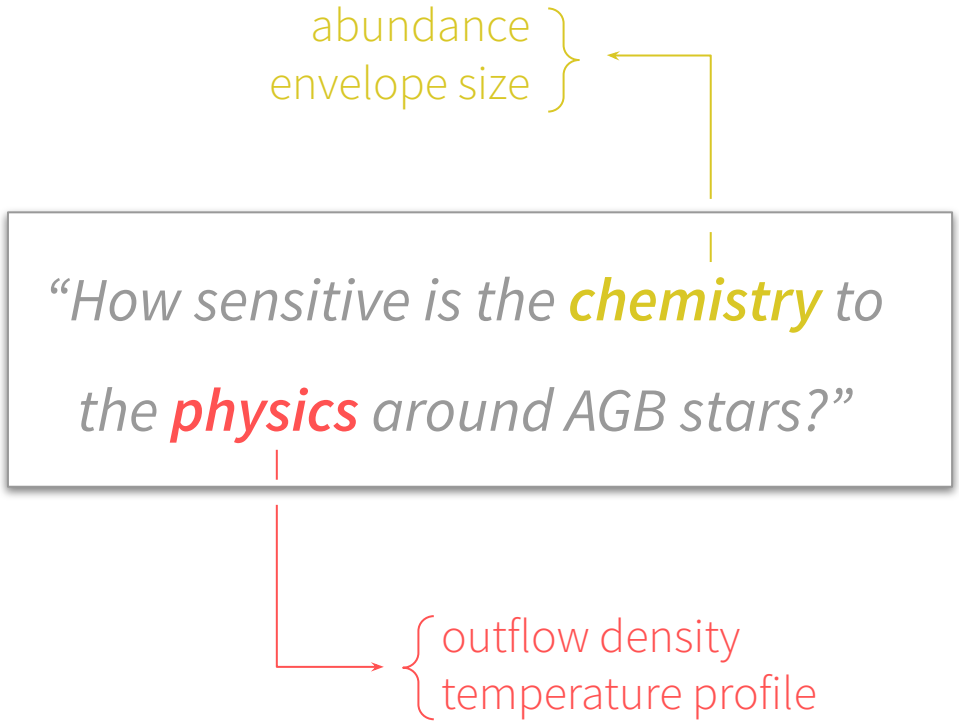
Source: M. Van de Sande

Aim

Aim

*"How sensitive is the **chemistry** to the **physics** around AGB stars?"*

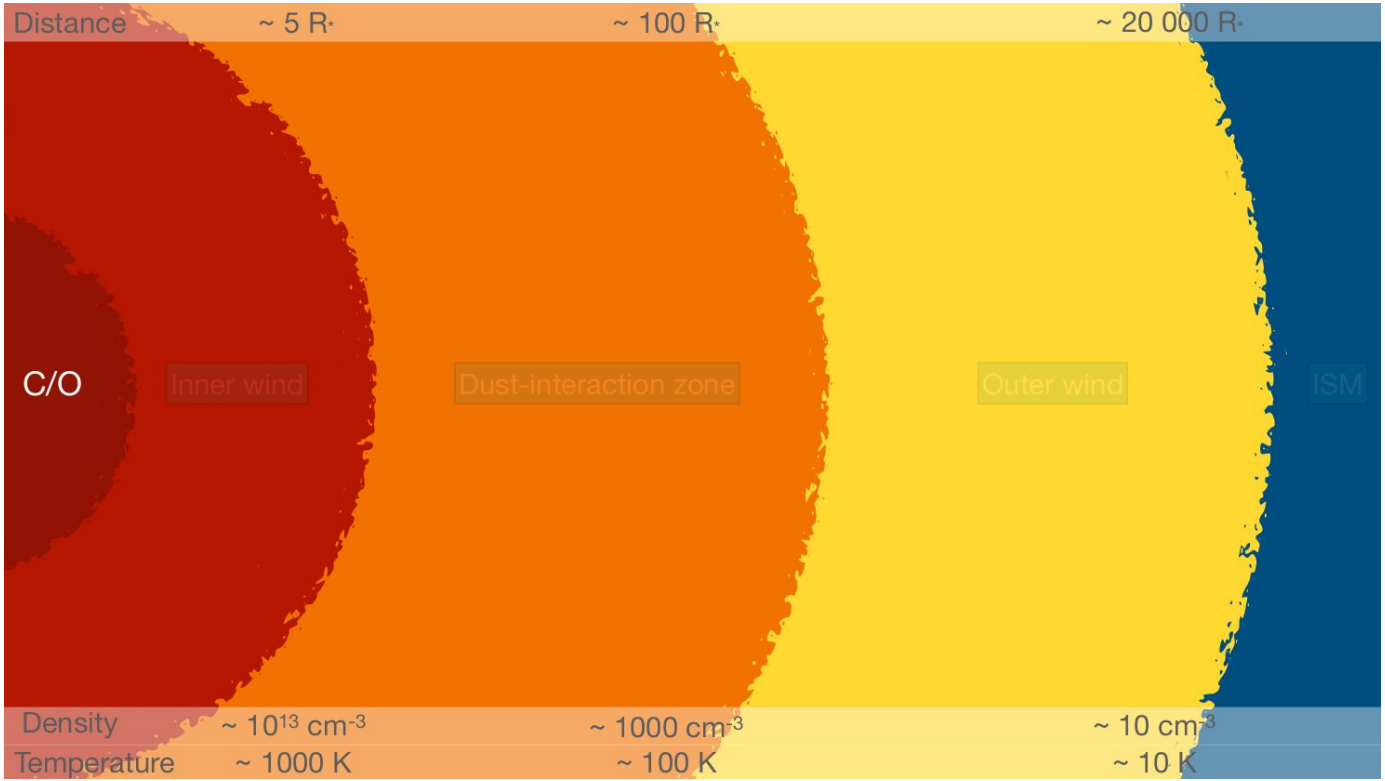
Aim


abundance
envelope size
"How sensitive is the chemistry to the physics around AGB stars?"
outflow density
temperature profile

Modelling

[1] based on *UMIST Database for Astrochemistry*

1D-CSE model[1]



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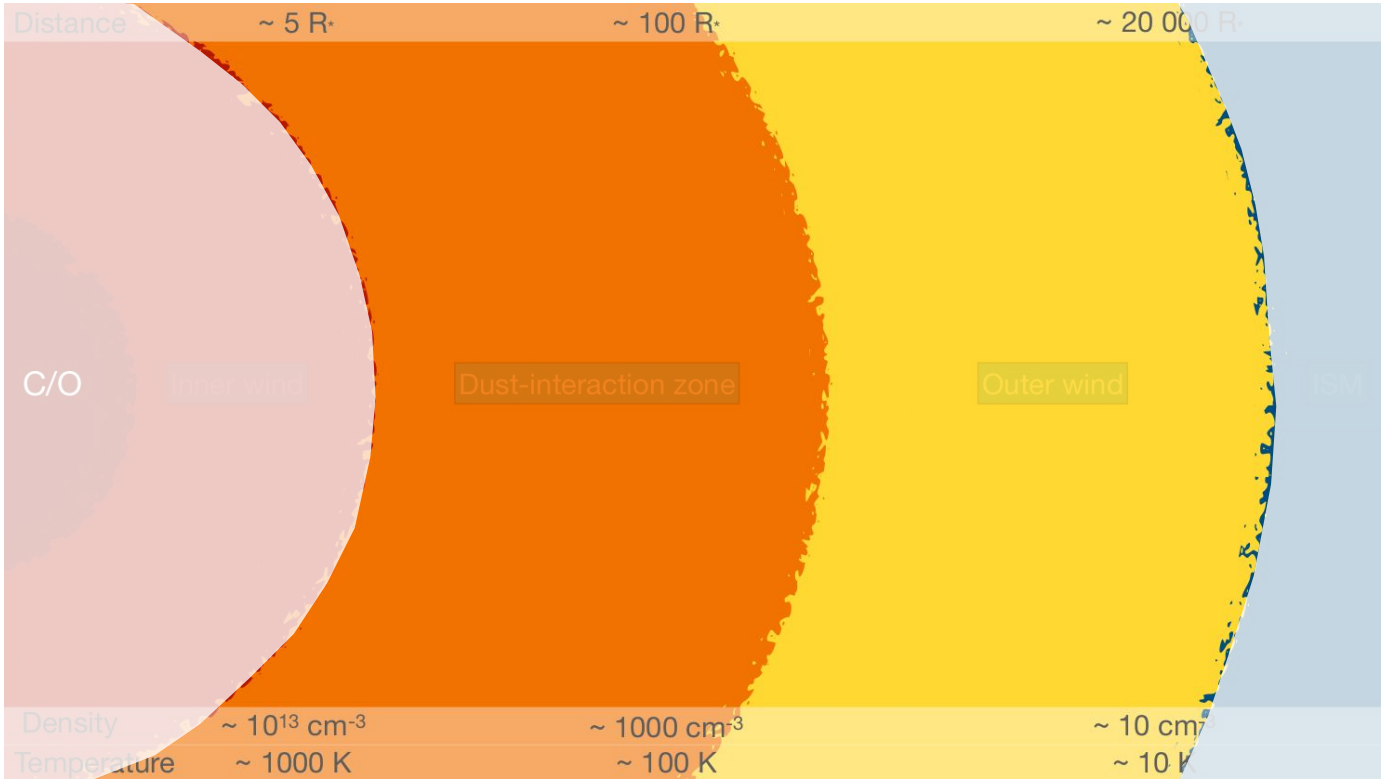

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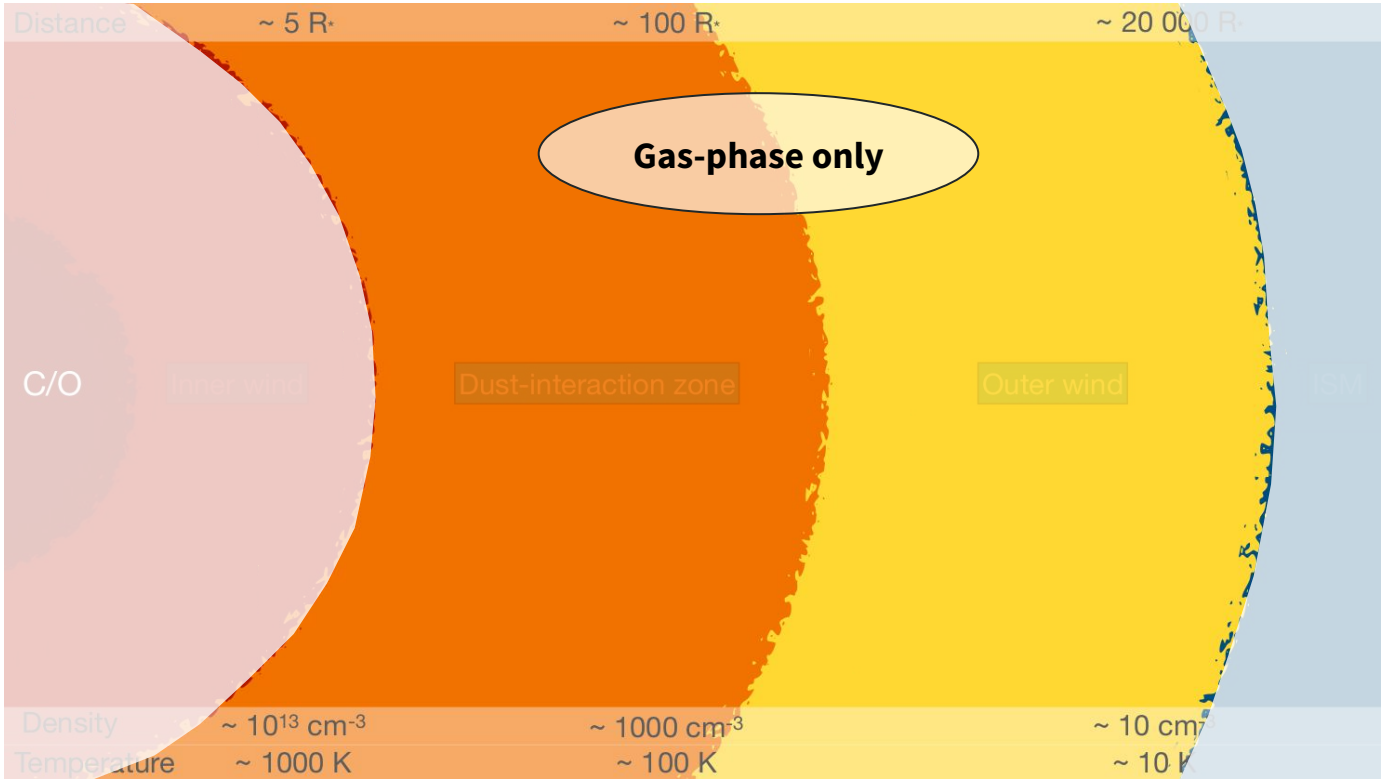

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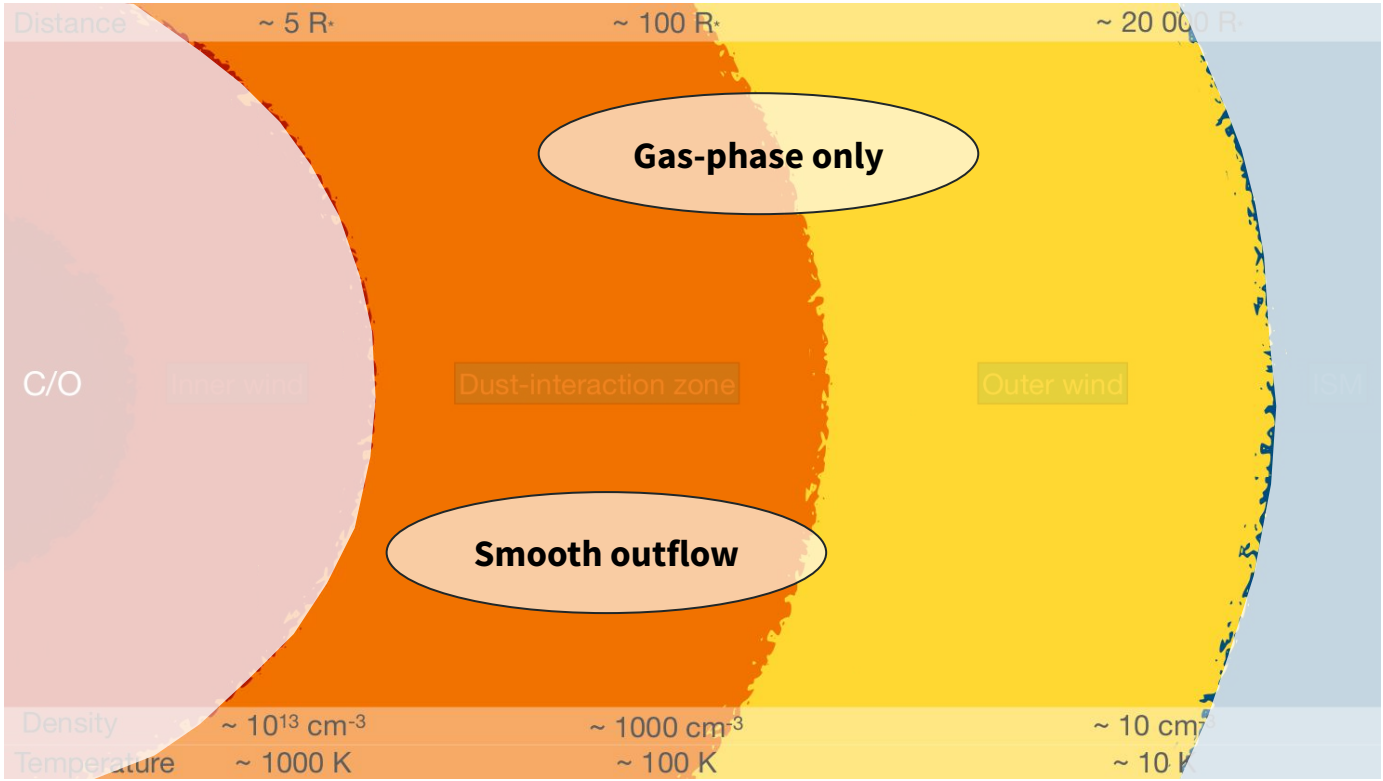

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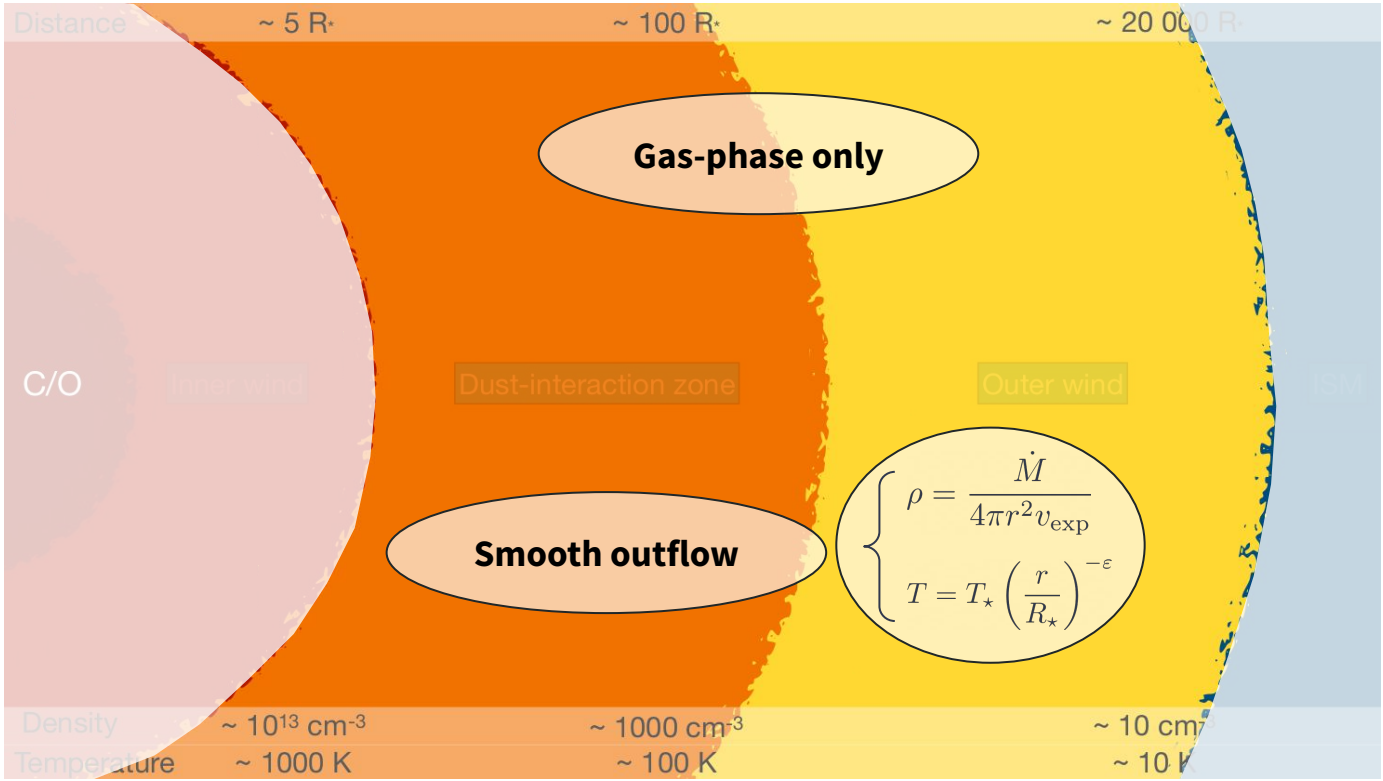

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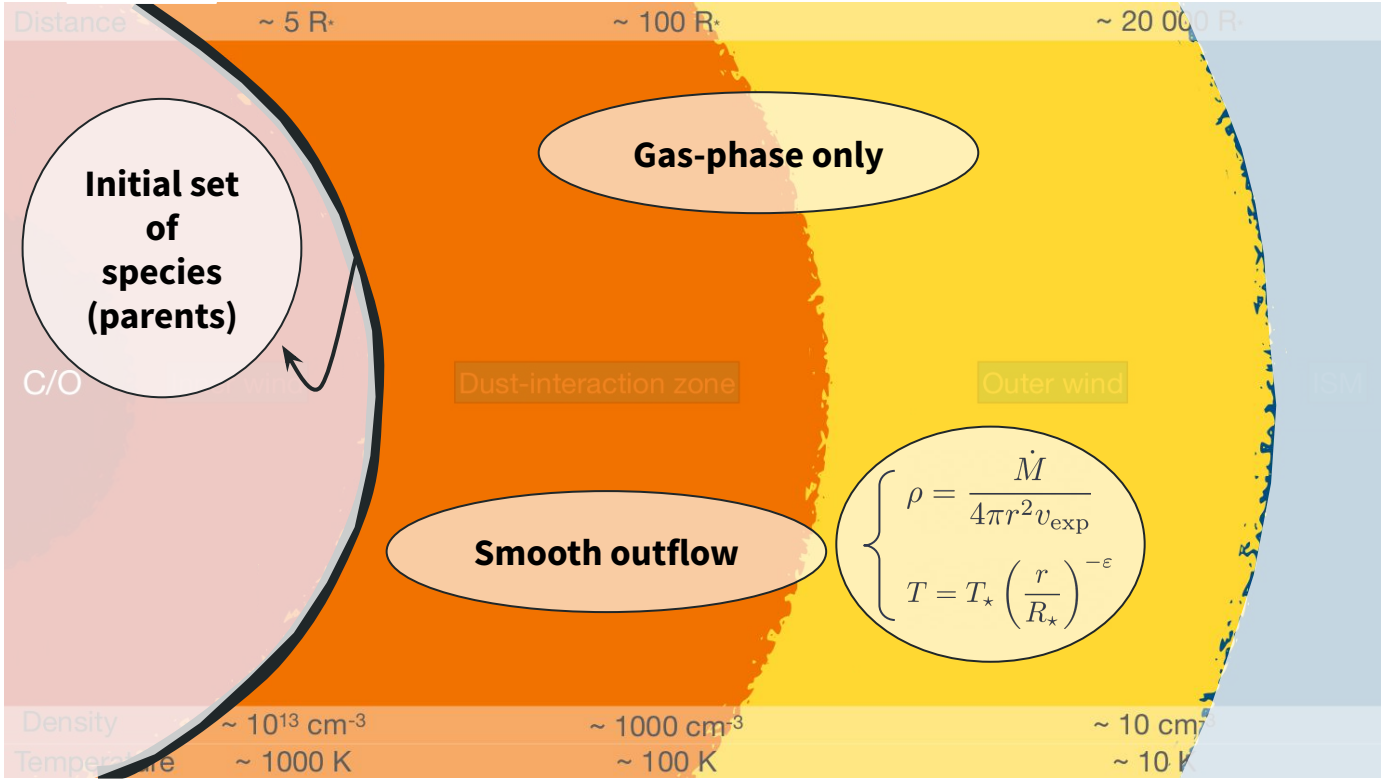

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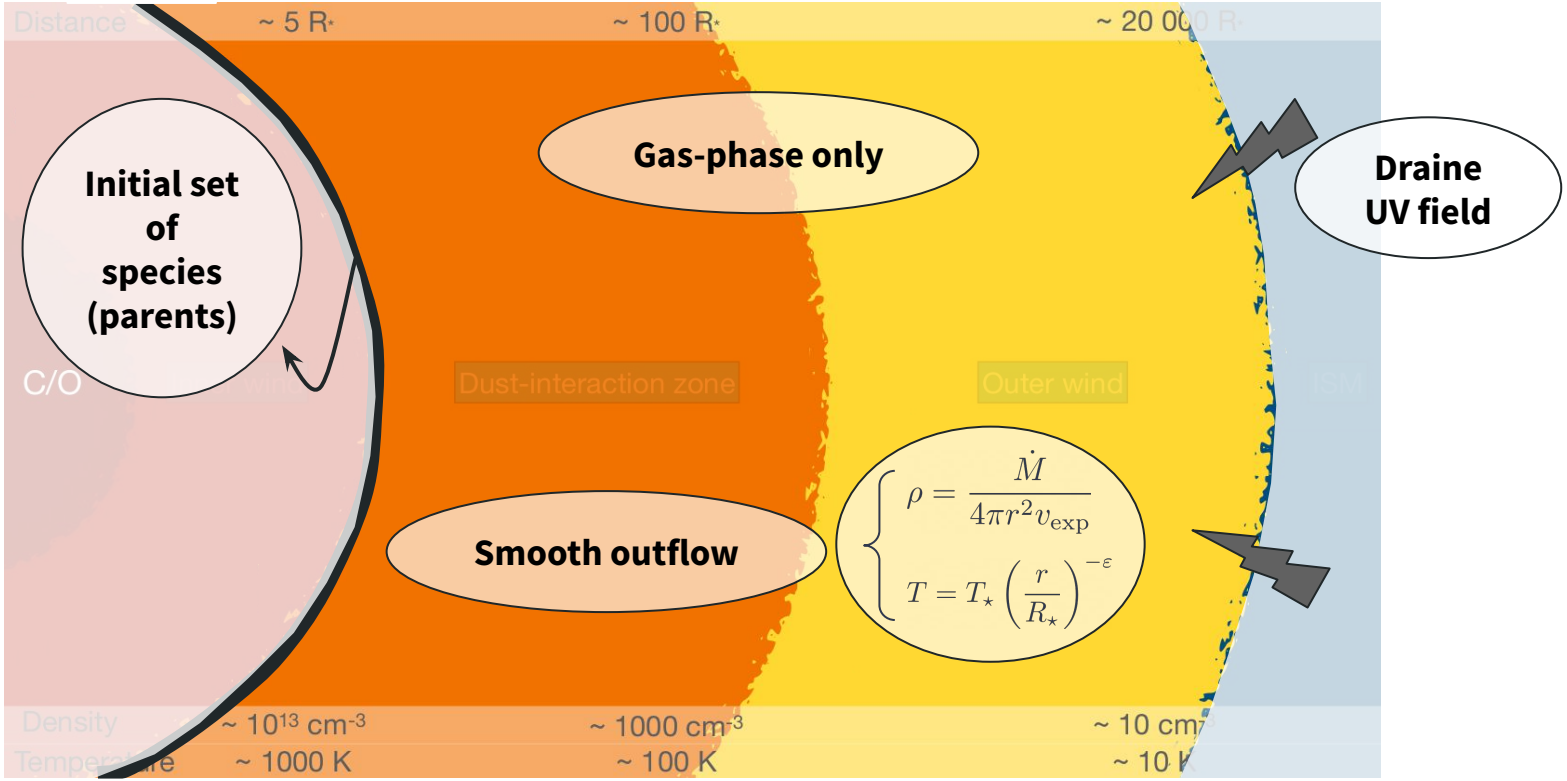

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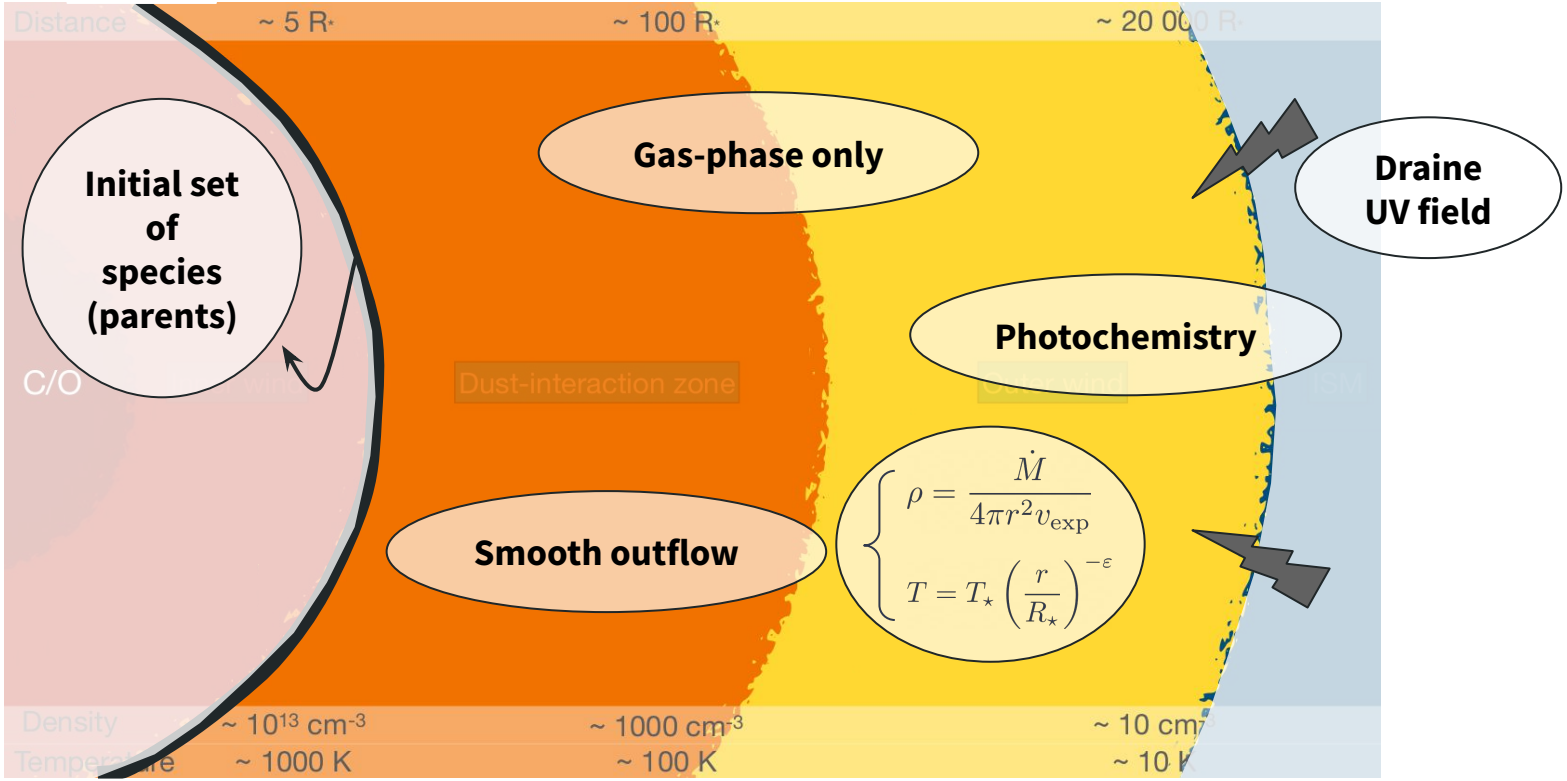

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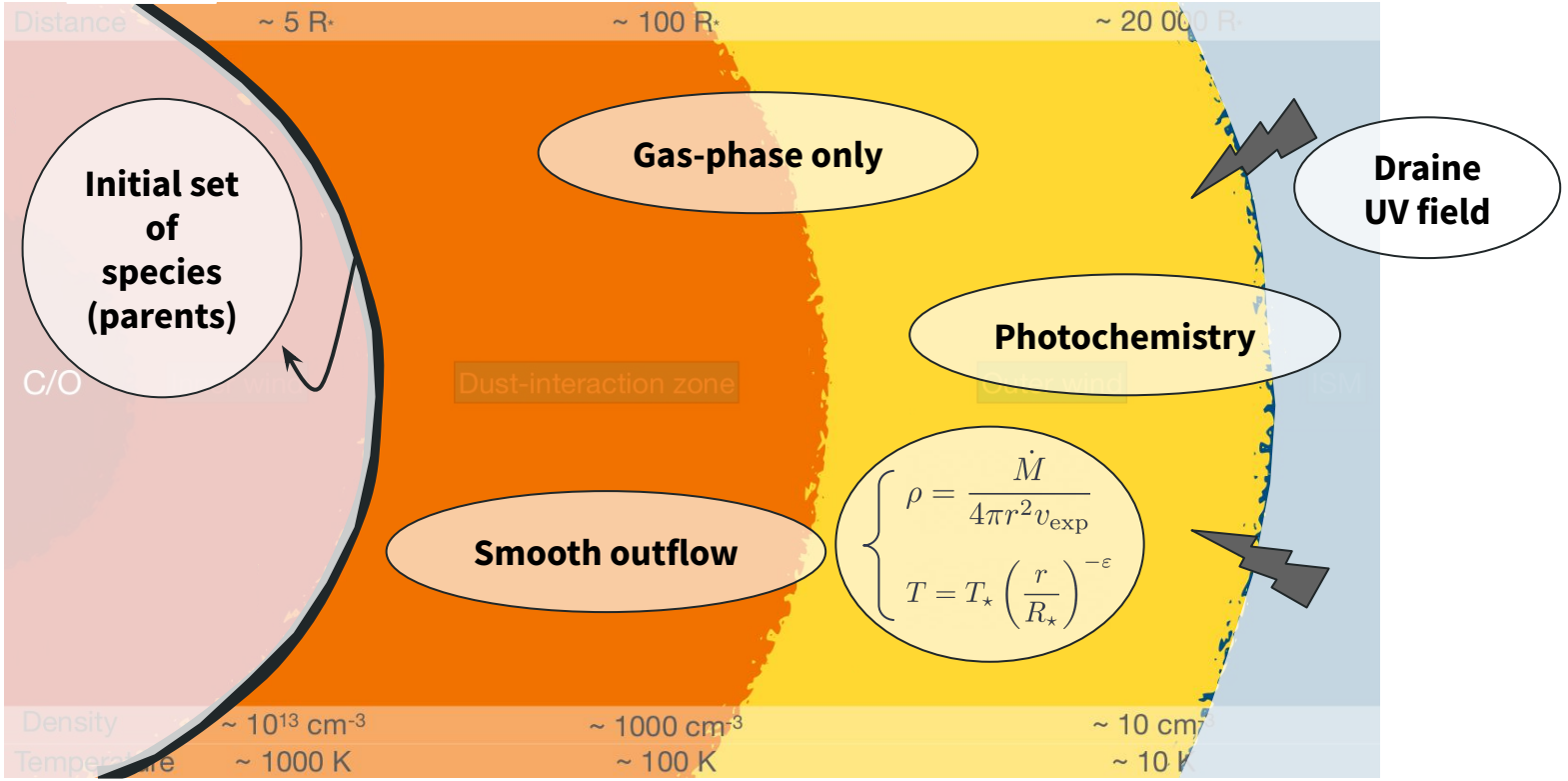
1D-CSE model[1]

Network:

Rate12[1]
(McElroy+ 2013)

~ 500 species

> 6000 reactions



Chemical kinetics

- *Non-equilibrium* thermodynamic & chemical conditions

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \sum_{j \in F_i} \left(k_j \prod_{r \in R_j} n_r \right) - \sum_{j \in D_i} \left(k_j \prod_{r \in R_j} n_r \right)$$

production reactions *destruction reactions*

Arrhenius law: $k = \alpha \left(\frac{T}{300\,\mathrm{K}} \right)^{\beta} \exp\left(\frac{-\gamma}{T} \right) \quad [\mathrm{cm}^3\,\mathrm{s}^{-1}]$

Grid

- *Input*:
  - mass-loss rate
  - expansion velocity

$$\rho = \frac{\dot{M}}{4\pi r^2 v_{\exp}}$$

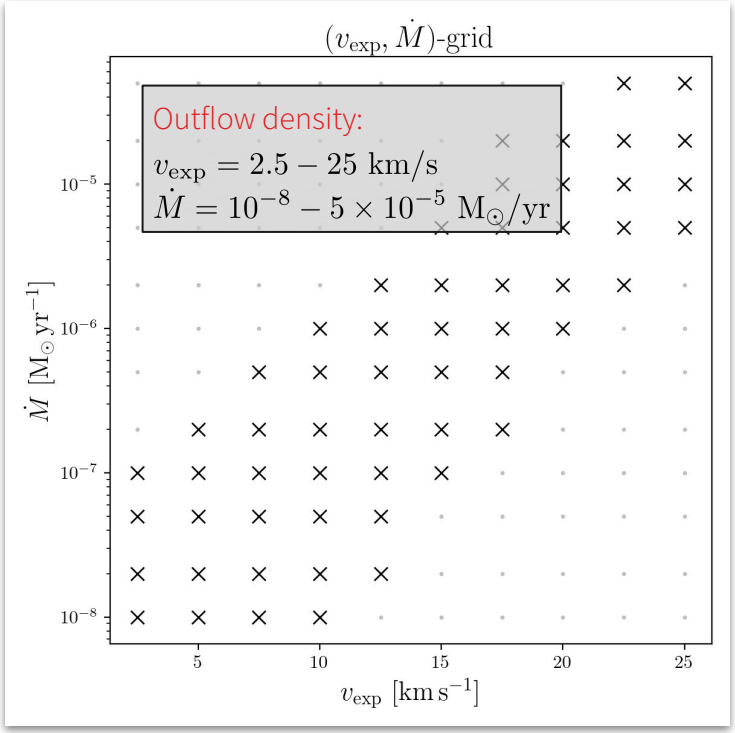
  - stellar temperature
  - temperature coefficient

$$T = T_\star \left(\frac{r}{R_\star}\right)^{-\varepsilon}$$

  - parent species: C-rich vs. O-rich

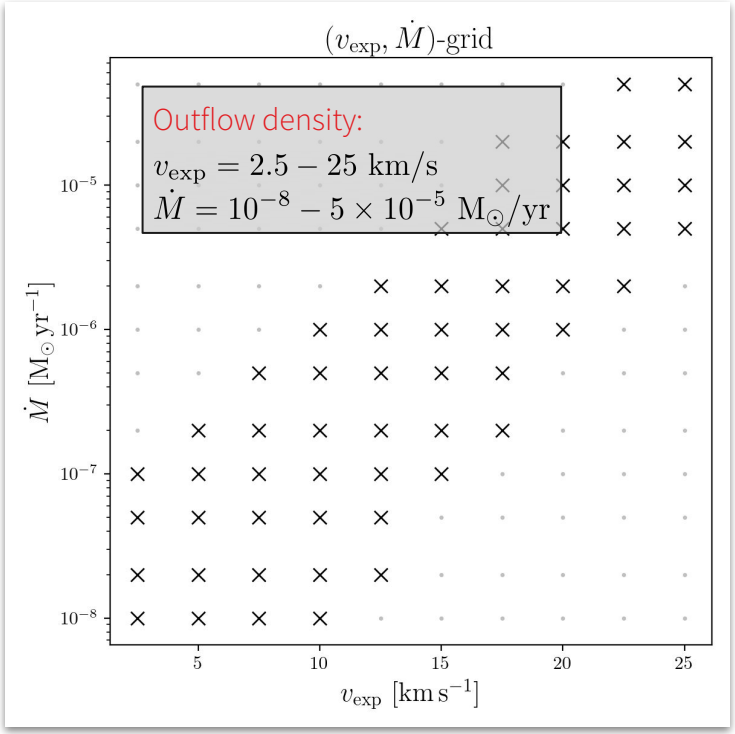
Carbon-rich		Oxygen-rich	
Species	Abundance	Species	Abundance
He	0.17	He	0.17
CO	8.00×10^{-4}	CO	3.00×10^{-4}
C_2H_2	4.38×10^{-5}	H_2O	2.15×10^{-4}
HCN	4.09×10^{-5}	N_2	4.00×10^{-5}
N_2	4.00×10^{-5}	SiO	2.71×10^{-5}
SiC_2	1.87×10^{-5}	H_2S	1.75×10^{-5}
CS	1.06×10^{-5}	SO_2	3.72×10^{-6}
H_2S	4.00×10^{-9}	SO	3.06×10^{-6}
NH_3	1.20×10^{-7}	SiS	9.53×10^{-7}
H_2O	2.55×10^{-6}	NH_3	6.25×10^{-7}
SiS	5.89×10^{-6}	CO_2	3.00×10^{-7}
SiO	5.02×10^{-6}	HCN	2.59×10^{-7}
CH_4	3.50×10^{-6}	PO	7.75×10^{-8}
HCl	3.25×10^{-7}	CS	5.57×10^{-8}
C_2H_4	6.85×10^{-8}	PN	1.50×10^{-8}
HCP	2.50×10^{-8}	Cl	1.00×10^{-8}
HF	1.70×10^{-8}	F	1.00×10^{-8}

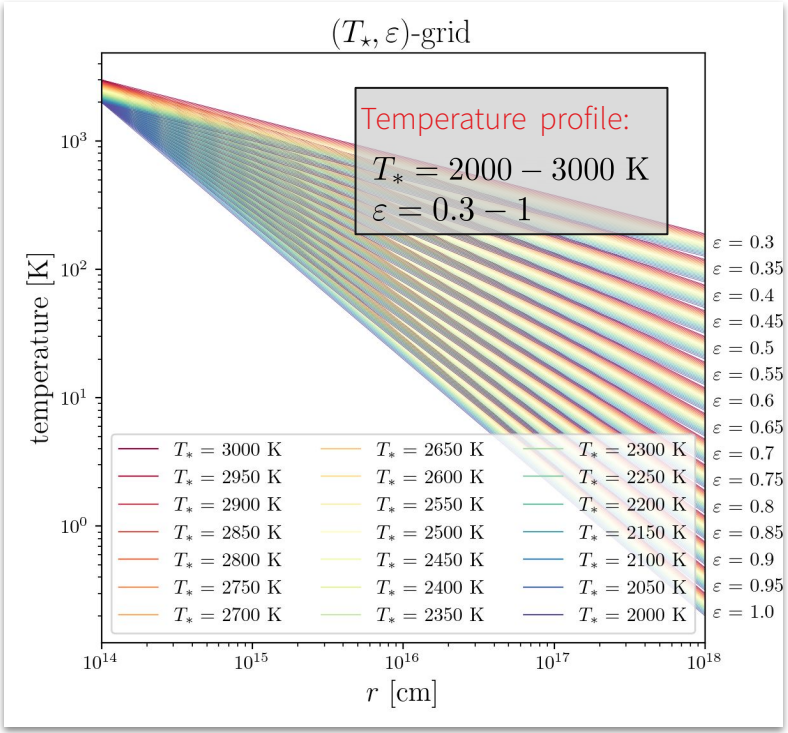
Grid


$(v_{\rm exp}, \dot{M})$-grid
Outflow density:
$v_{\rm exp} = 2.5 - 25$ km/s
$\dot{M} = 10^{-8} - 5 \times 10^{-5}$ M$_\odot$/yr
10^{-5}
10^{-6}
10^{-7}
10^{-8}
$\dot{M}$ [M$_\odot$ yr^{-1}]
5
10
15
20
25
$v_{\rm exp}$ [km s^{-1}]

Grid

Total number of models: ***34 020***





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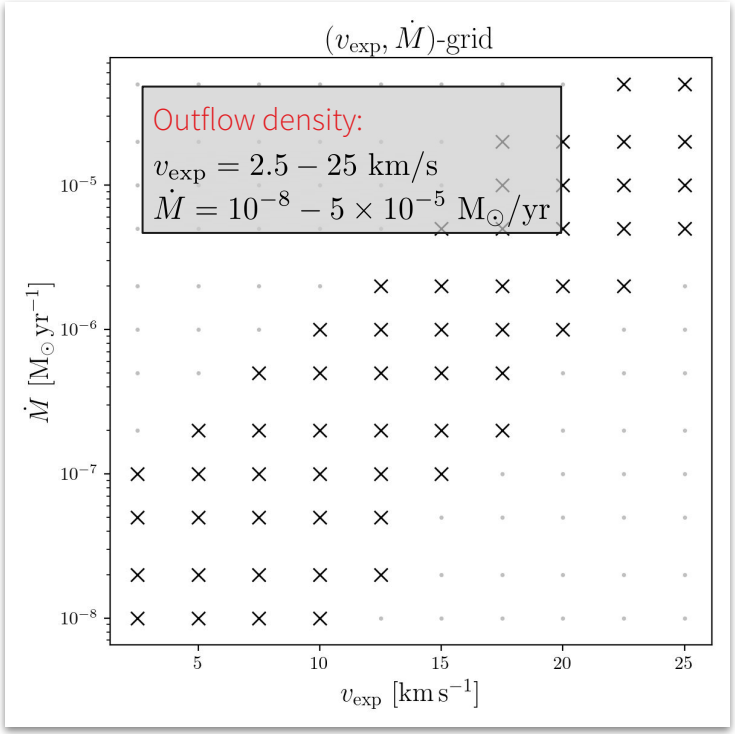
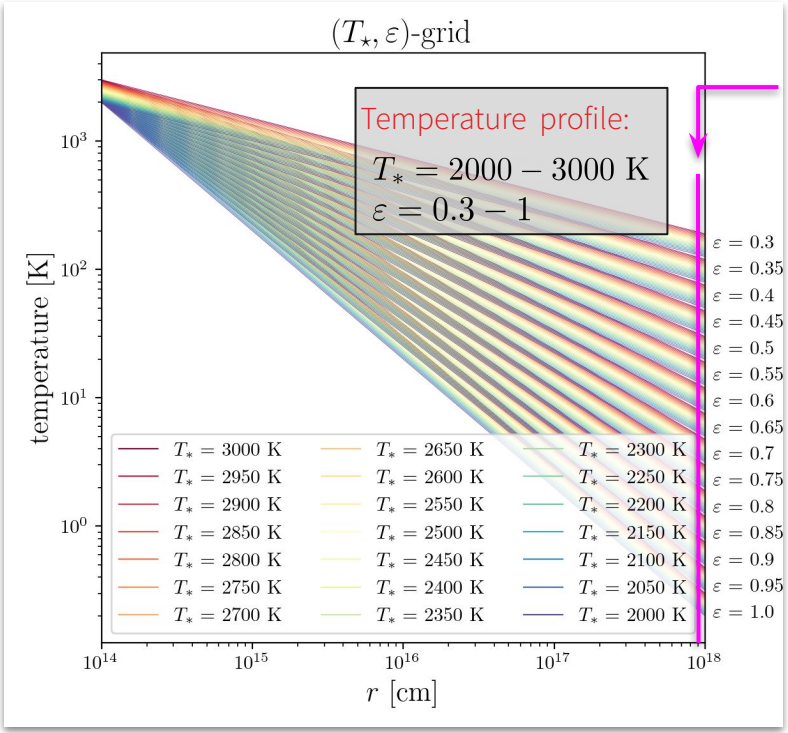
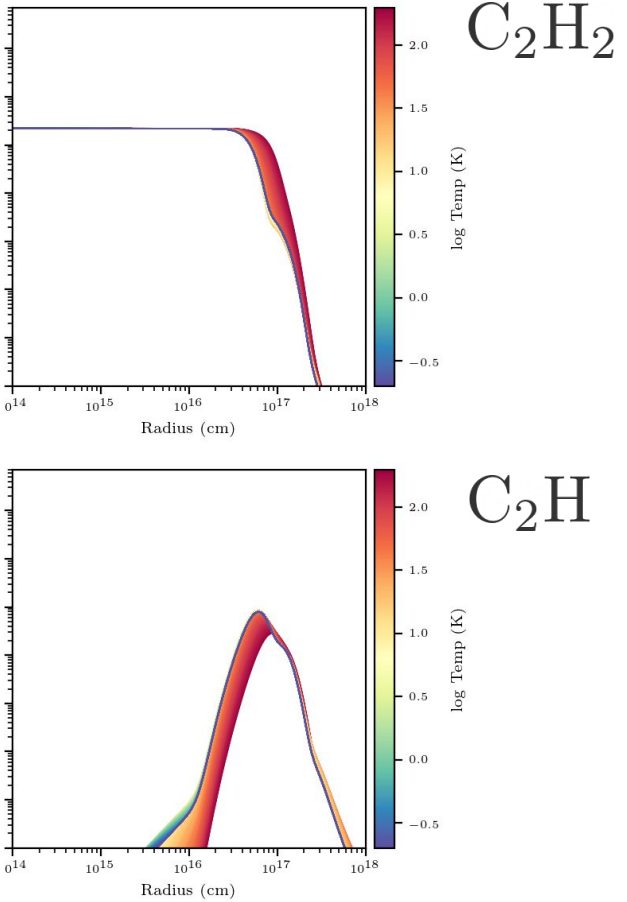




reference temperature

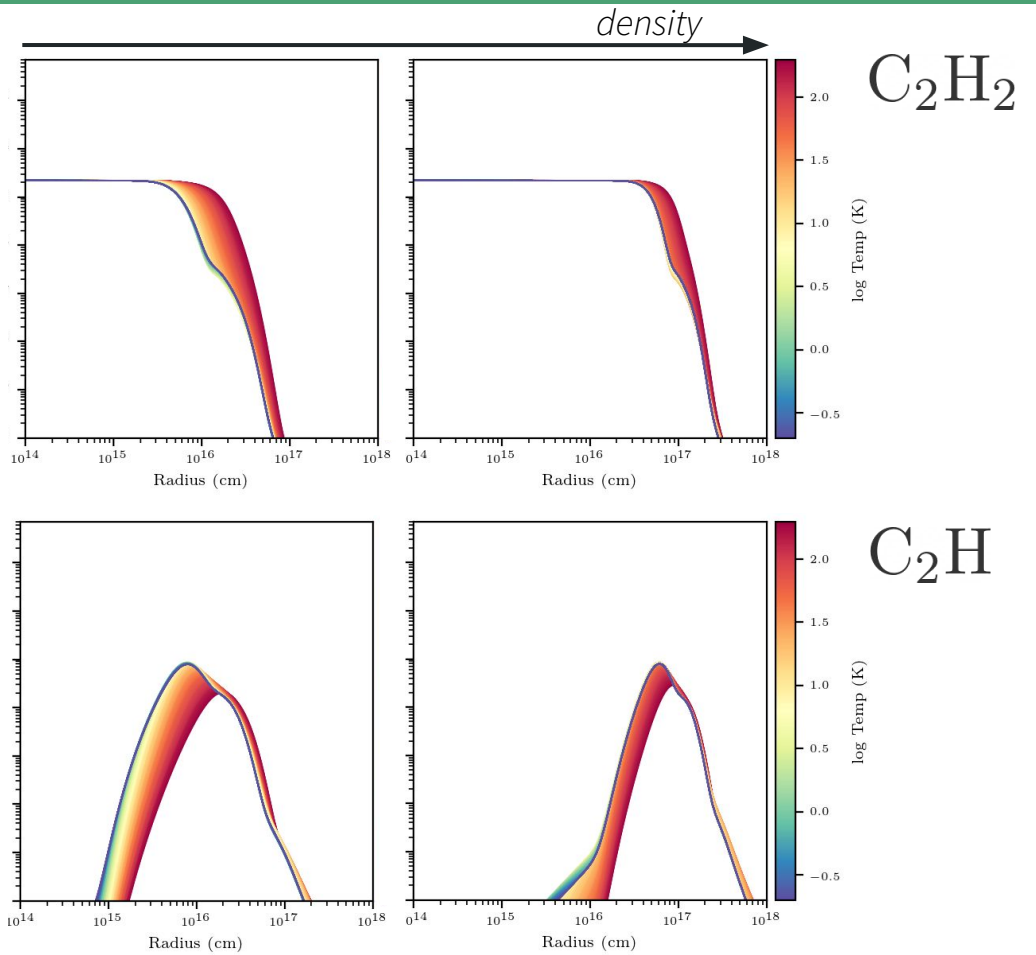
Results: sensitivity study

Results



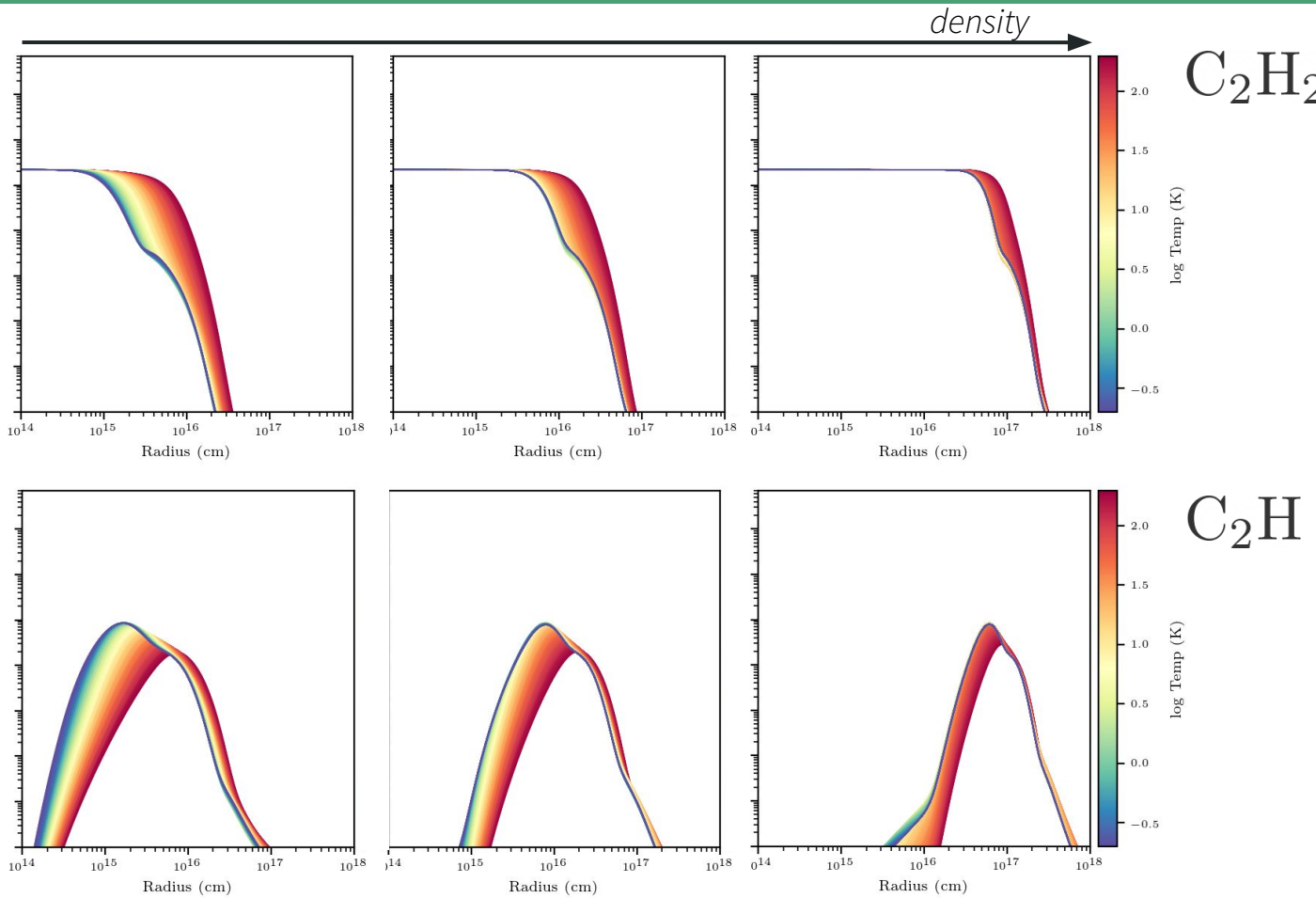
C-rich outflow

Results



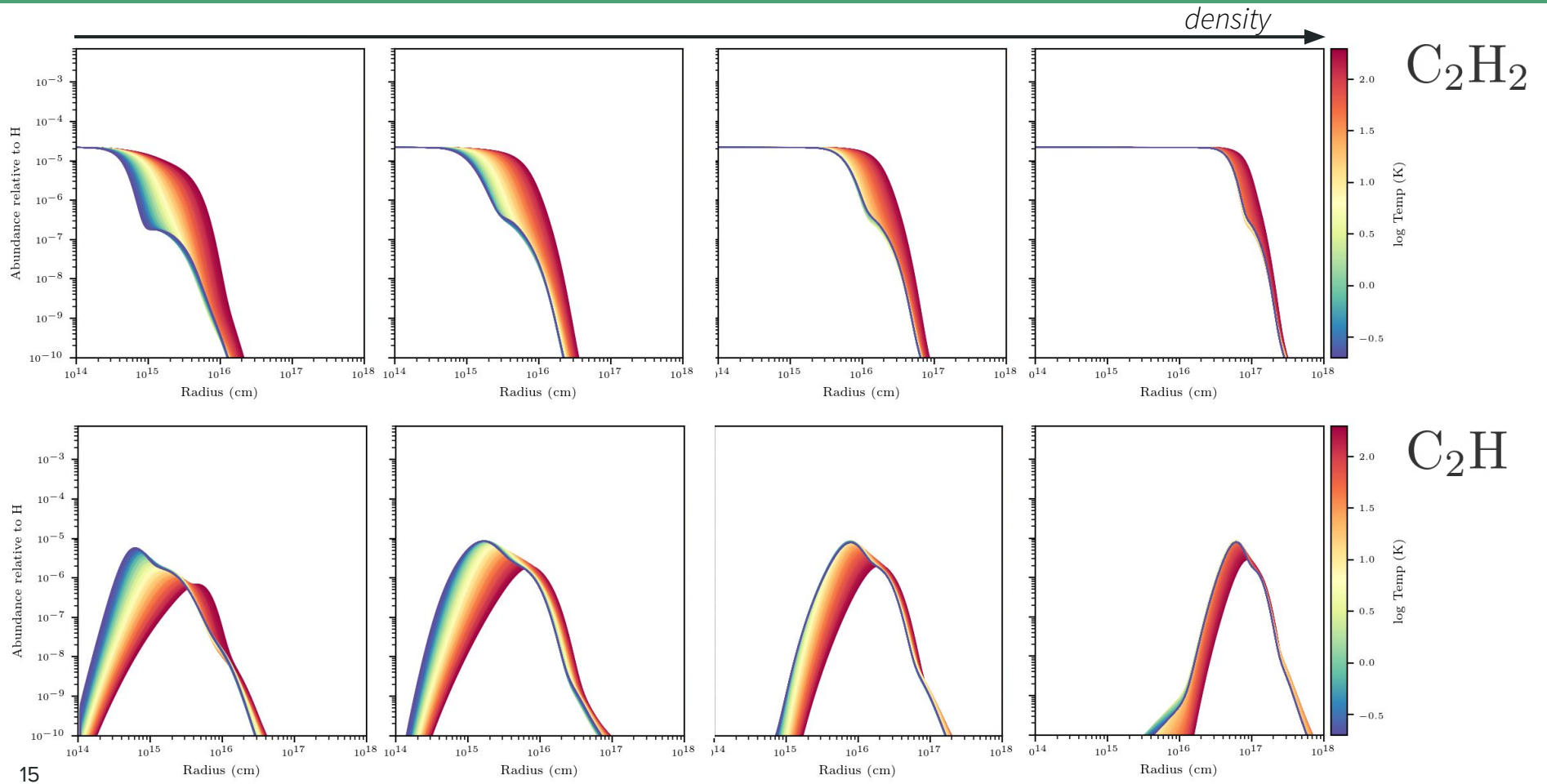
C-rich outflow

Results



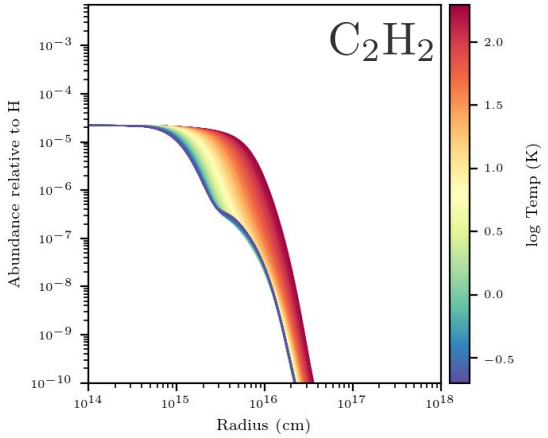
C-rich outflow

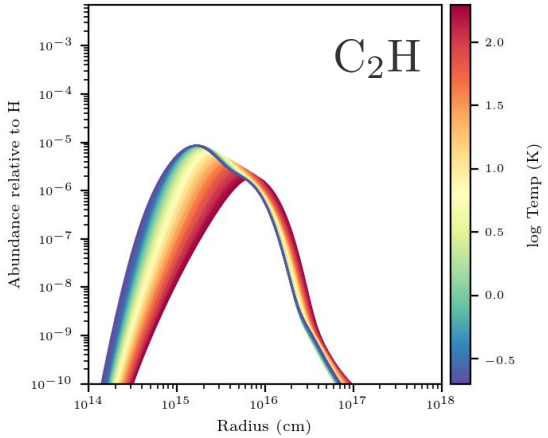
Sensitivity study



Results

Energy barrier



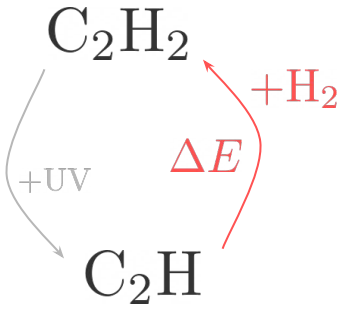


C-rich outflow

Arrhenius Law:

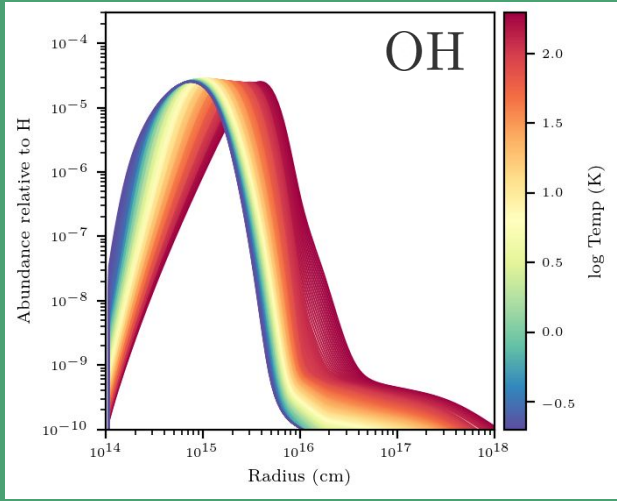
$$k = \alpha \left(\frac{T}{300\,\mathrm{K}}\right)^{\beta} \exp\left(\frac{-\gamma}{T}\right) \quad [\mathrm{cm^3\,s^{-1}}]$$

Network:



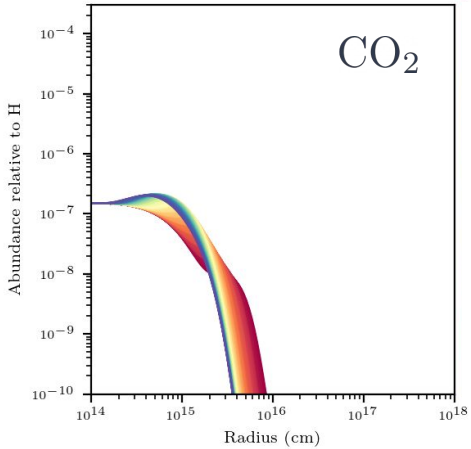
Results

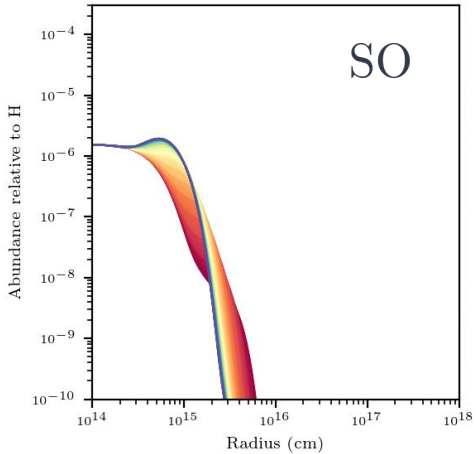
"Inheriting" of profiles



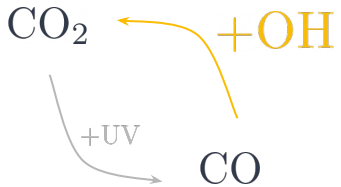
O-rich outflow

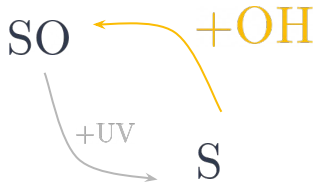
Sensitivity study





Network:





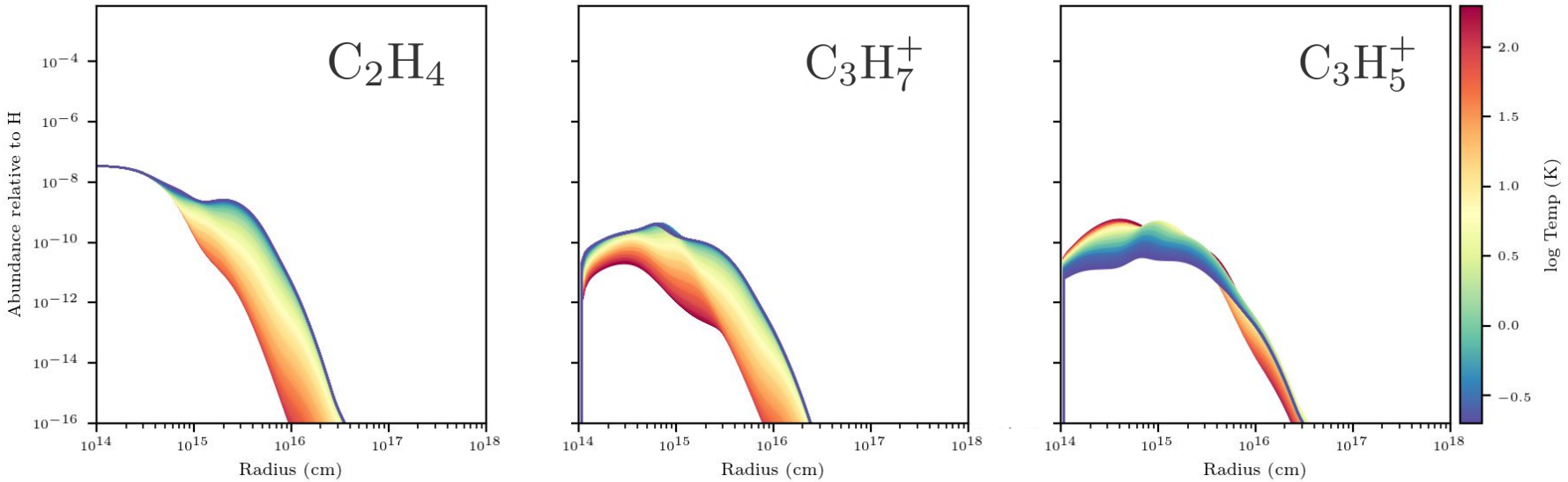
Results

$$k = \alpha \left(\frac{T}{300\,\mathrm{K}}\right)^{\beta} \exp\left(\frac{-\gamma}{T}\right) \quad [\mathrm{cm^3\,s^{-1}}]$$

Negative beta-exponent

$\beta = -2.9$

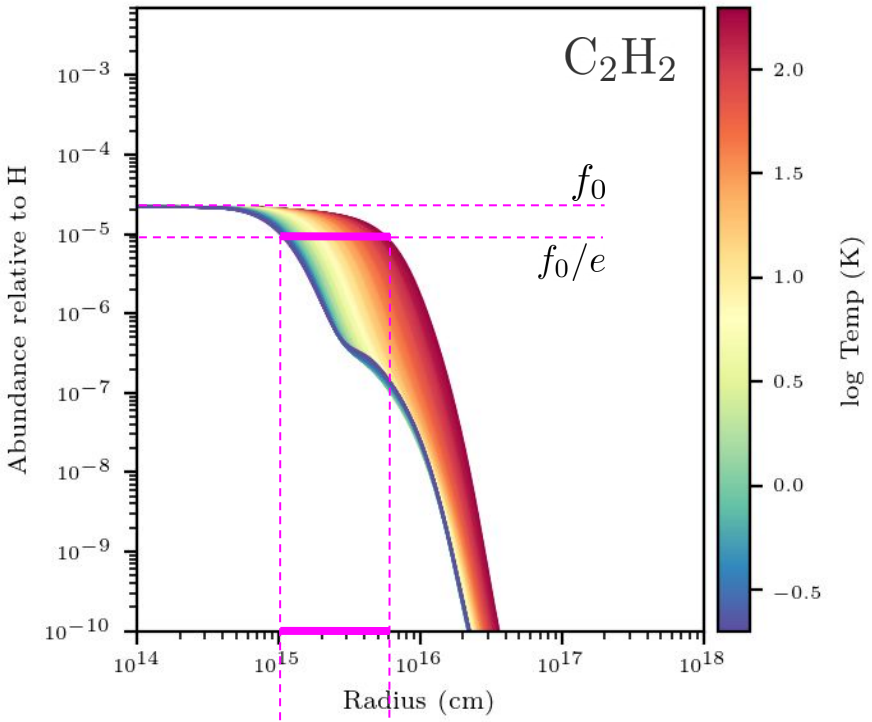
$+e^-$ $+H_2$



C-rich outflow

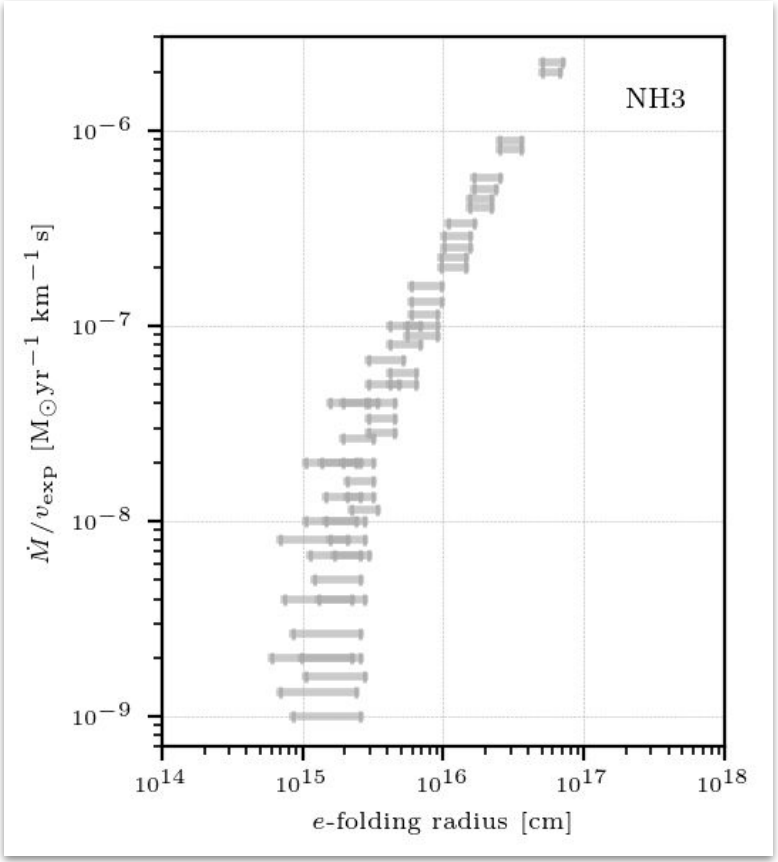
Envelope sizes

e-folding radius



C-rich outflow

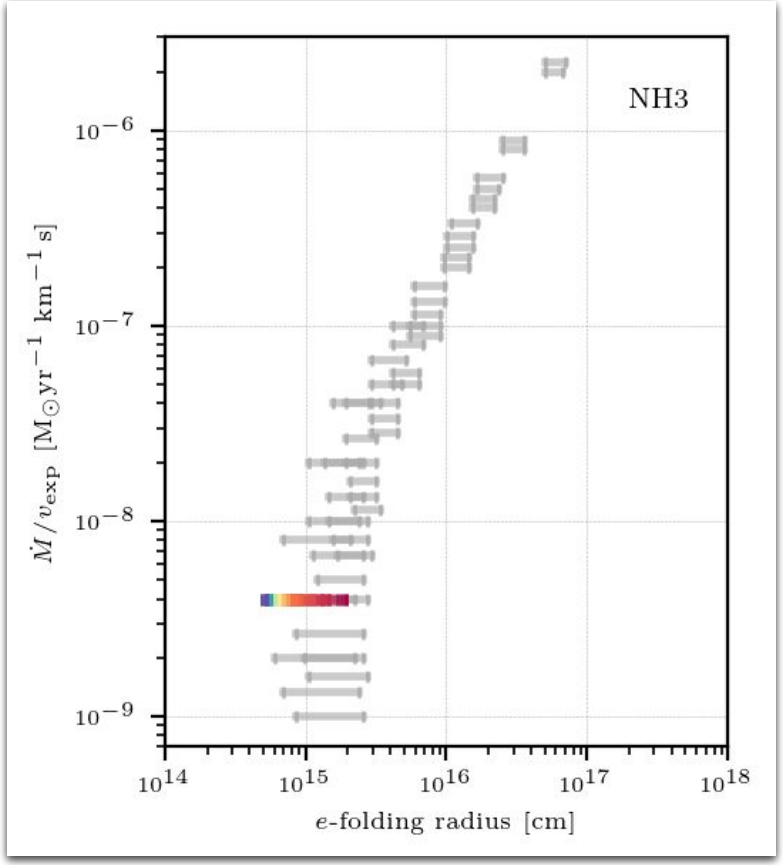
Envelope sizes



C-rich outflow

Envelope sizes

- ***Temperature variation*** per density



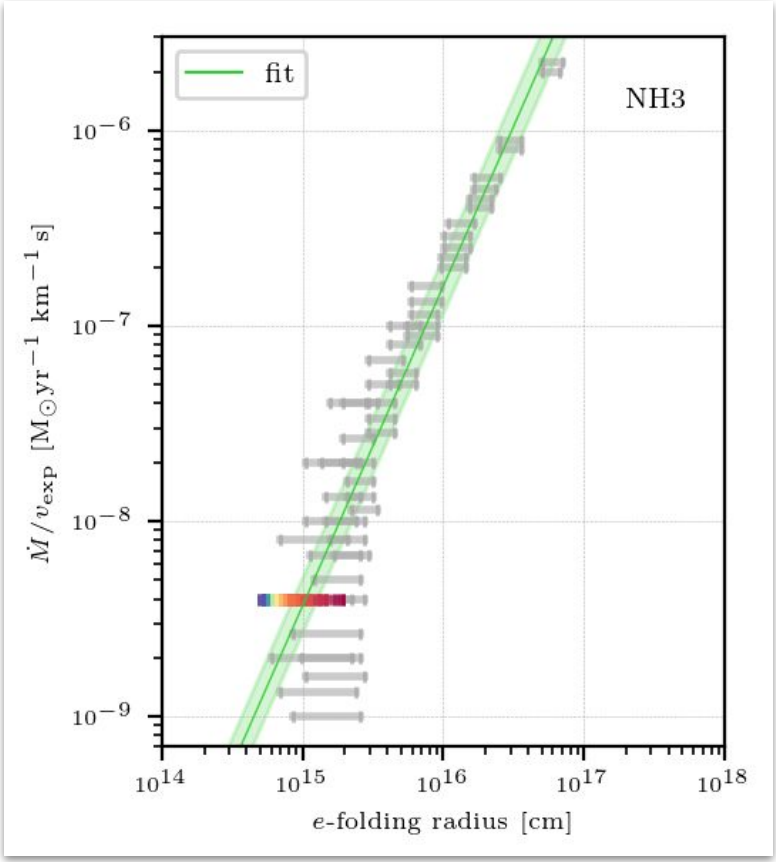
C-rich outflow

Envelope sizes

- ***Temperature variation*** per density

- *Linear relation* → fit in log-scale

$$\log \frac{\dot{M}}{v_{\rm exp}} = a \log R_e + b$$



C-rich outflow

Envelope sizes

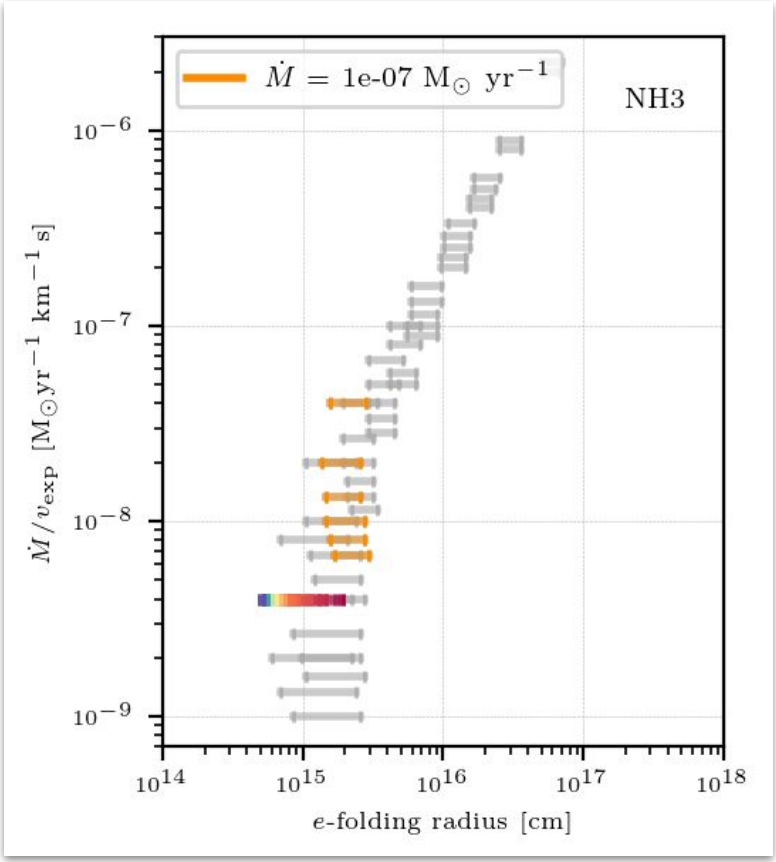
- ***Temperature variation*** per density

- *Linear relation* → fit in log-scale

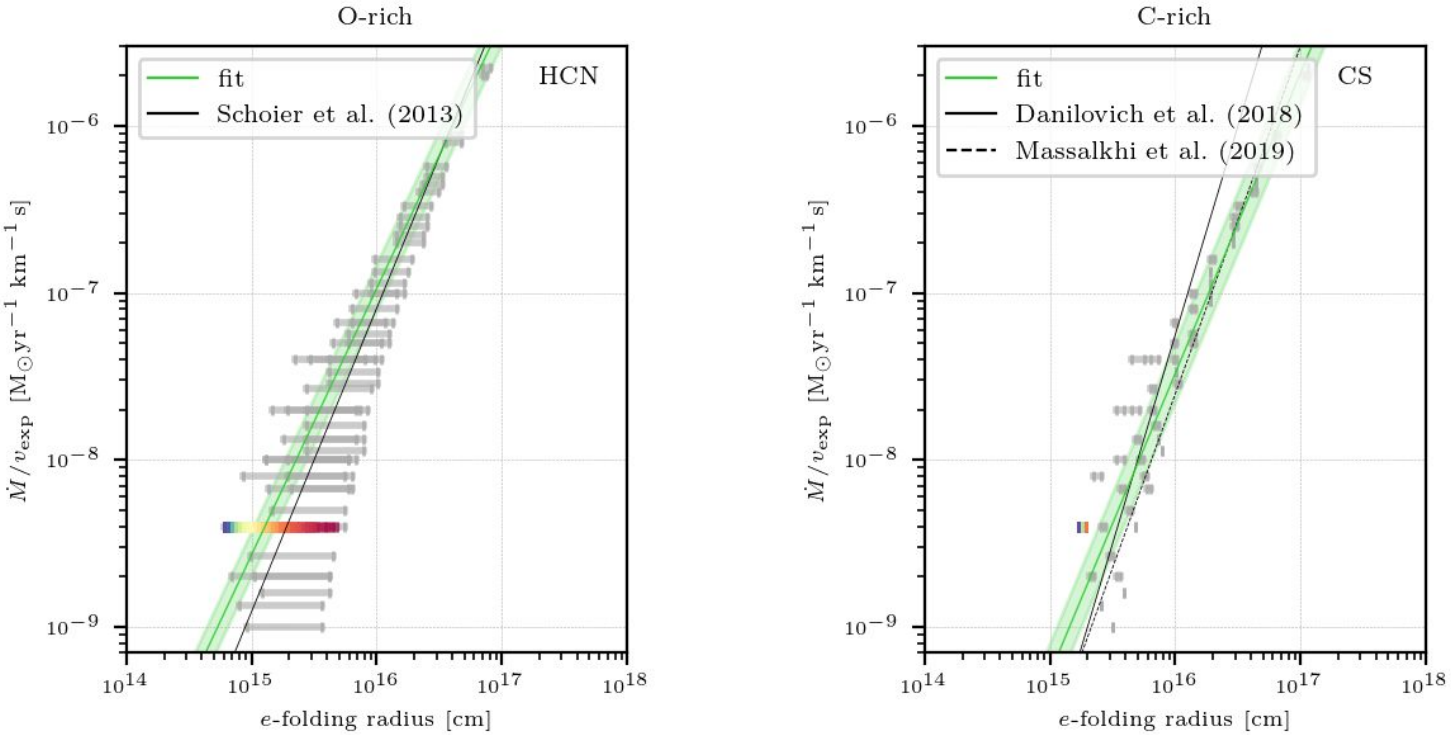
- Effect of *CO self-shielding*:

  dependent of expansion velocity

$$\rho = \frac{\dot{M}}{4\pi r^2 v_{\rm exp}}$$



Envelope sizes: comparison to literature/observations



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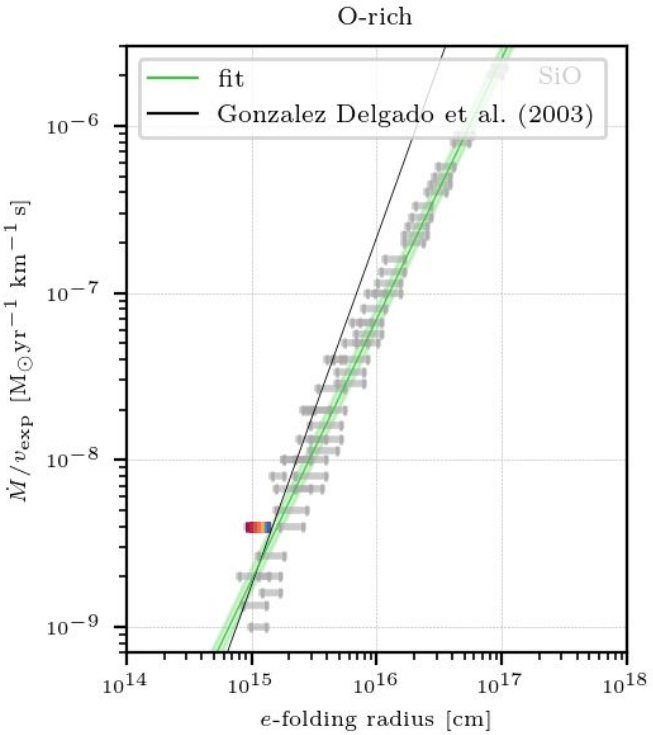
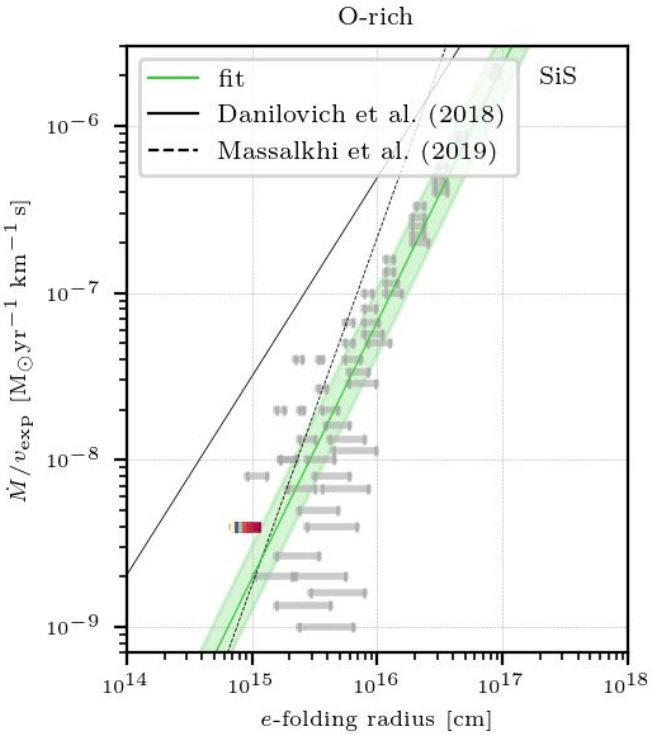


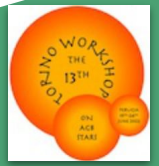


Conclusions

- Abundances vary with { density, temperature } → - energy barrier
  - ‘inheritance’
  - beta < 0

- Missing chemistry for SiS?

→ chemical thermometer?



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Conclusions

- Abundances vary with { density / temperature → - energy barrier / - ‘inheritance’ / - beta < 0

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→ ***chemical thermometer?***

Thank you!

Contact:
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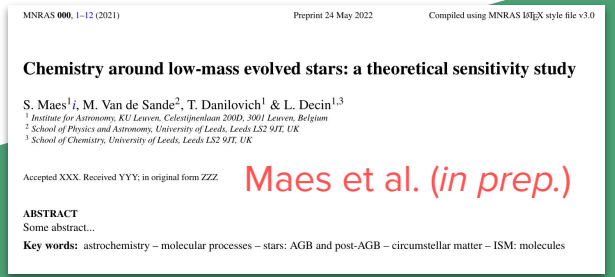

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Chemistry around low-mass evolved stars: a theoretical sensitivity study

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ABSTRACT
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